ELSEVIER

Chemical Physics 224 (1997) 337–339

Chemical Physics

Author index to volume 224

Agreiter, J., M. Lorenz, A.M. Smith and V.E. Bondybey, Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2 224 (1997) 301
Ågren, H., see Jonsson, D. 224 (1997) 201

Bagryanskaya, E.G., see Gorelik, V.R. 224 (1997) 229
Baltzer, P., L. Karlsson, B. Wannberg, G. Öhrwall, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and W. von Niessen, An experimental and theoretical study of the valence shell photoelectron spectrum of the benzene molecule 224 (1997) 95
Billing, G.D., see Marković, N. 224 (1997) 53
Billing, G.D., see Wang, L. 224 (1997) 65
Bleyer, A., see Holzer, W. 224 (1997) 315
Bondybey, V.E., see Agreiter, J. 224 (1997) 301
Bradley, D.D.C., see Holzer, W. 224 (1997) 315
Brady, J.W., see Naidoo, K.J. 224 (1997) 263

Chau, F.-T., J.M. Dyke, E.P.F. Lee, A. Ridha and D.-C. Wang, HeI photoelectron spectra of PH_2 and PF_2: comparison between simulation and experiment 224 (1997) 157
Chesnut, D.B., Ab initio NMR chemical shieldings in the neutral and charged 7-phosphabicyclo[2.2.1]heptane, -heptene, and -heptadiene systems; the largest predicted downfield shift for a conventional organophosphorus molecule 224 (1997) 133

Dézarnaud-Dandine, C., see Guillot, F. 224 (1997) 281
Ding, S., see Guan, D. 224 (1997) 243
Dolg, M., see Yu, M. 224 (1997) 121
Dyke, J.M., see Chau, F.-T. 224 (1997) 157
Dyson, A.J., see Solca, J. 224 (1997) 253

Friedrich, J., see Köhler, M. 224 (1997) 327

Gehlen, M.H., Spectral analysis of the fluorescence quenching kinetics in micelles with probe migration 224 (1997) 275
Gong, S.-H., see Holzer, W. 224 (1997) 315
Gorelik, V.R., V.A. Morozov, N.N. Lukzen, E.G. Bagryanskaya and R.Z. Sagdeev, The manifestation of degenerate electron exchange in stimulated nuclear polarization at high magnetic fields 224 (1997) 229
Grein, F., see Hachey, M.R.J. 224 (1997) 19
Grimme, S., see Pulm, F. 224 (1997) 143
Guan, D., X. Yi, S. Ding, B. Yang and J.A. Olson, A theoretical treatment for the dynamics of near-resonant charge exchange in gas–surface scattering 224 (1997) 243

Guillot, F., C. Dézarnaud-Dandine and M. Tronc, X-ray absorption study of potential barrier effect in group 14 tetrachlorides ($GeCl_4$, $SnCl_4$) and group 15 trichlorides (PCl_3, $AsCl_3$) 224 (1997) 281

Hachey, M.R.J. and F. Grein, Multireference configuration-interaction studies on the UV and photoelectron spectrum of phosgene, Cl_2CO 224 (1997) 19
Hayes, M.A., see Baltzer, P. 224 (1997) 95
Holland, D.M.P., see Baltzer, P. 224 (1997) 95
Holzer, W., A. Penzkofer, S.-H. Gong, D.D.C. Bradley, X. Long and A. Bleyer, Effective stimulated emission and excited-state absorption cross-section spectra of poly(m-phenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) and t,t′-didecyloxy-II-distyrylbenzene 224 (1997) 315
Hormes, J., see Pulm, F. 224 (1997) 143
Huber, H., see Solca, J. 224 (1997) 253

Jonsson, D., P. Norman and H. Ågren, Single determinant calculations of excited state polarizabilities 224 (1997) 201

Kalvoda, S., see Yu, M. 224 (1997) 121
Karlsson, L., see Baltzer, P. 224 (1997) 95
Kirchner, B., see Solca, J. 224 (1997) 253
Knudson, S.K. and I.C. Palmer, Semiclassical electronic eigenvalues for charge asymmetric one-electron diatomic molecules: general method and sigma states 224 (1997) 1
Köhler, M., J. Friedrich, M. Laberge and J.M. Vanderkooi, Influence of the pH on the pocket field of cytochrome *c* type proteins 224 (1997) 327
Kristyán, S., Immediate estimation of correlation energy for molecular systems from the partial charges on atoms in the molecule 224 (1997) 33

Laberge, M., see Köhler, M. 224 (1997) 327
Lahaye, M., see You, L. 224 (1997) 81
Lee, E.P.F., P. Mack and T.G. Wright, The geometric structure and stability of the $NO^+ \cdot CH_4$ cationic complex 224 (1997) 191
Lee, E.P.F., see Chau, F.-T. 224 (1997) 157
Liu, Q., see You, L. 224 (1997) 81
Long, X., see Holzer, W. 224 (1997) 315
Lorenz, M., see Agreiter, J. 224 (1997) 301
Lukzen, N.N., see Gorelik, V.R. 224 (1997) 229

MacDonald, M.A., see Baltzer, P. 224 (1997) 95
Mack, P., see Lee, E.P.F. 224 (1997) 191
Marković, N. and G.D. Billing, Semi-classical treatment of chemical reactions: extension to 3D wave packets 224 (1997) 53
Morozov, V.A., see Gorelik, V.R. 224 (1997) 229
Muñoz-Crego, C. and J. Santamaría, Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution 224 (1997) 215

Naidoo, K.J. and J.W. Brady, The application of simulated annealing to the conformational analysis of disaccharides 224 (1997) 263
Norman, P., see Jonsson, D. 224 (1997) 201

Öhrwall, G., see Baltzer, P. 224 (1997) 95
Olson, J.A., see Guan, D. 224 (1997) 243

Palmer, I.C., see Knudson, S.K. 224 (1997) 1
Penzkofer, A., see Holzer, W. 224 (1997) 315
Peyerimhoff, S.D., see Pulm, F. 224 (1997) 143
Pulm, F., J. Schramm, J. Hormes, S. Grimme and S.D. Peyerimhoff, Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones 224 (1997) 143

Ridha, A., see Chau, F.-T. 224 (1997) 157

Sagdeev, R.Z., see Gorelik, V.R. 224 (1997) 229
Santamaría, J., see Muñoz-Crego, C. 224 (1997) 215
Schirmer, J., see Trofimov, A.B. 224 (1997) 175
Schramm, J., see Pulm, F. 224 (1997) 143
Shi, Y., see You, L. 224 (1997) 81
Smith, A.M., see Agreiter, J. 224 (1997) 301
Solca, J., A.J. Dyson, G. Steinebrunner, B. Kirchner and H. Huber, Melting curve for argon calculated from pure theory 224 (1997) 253
Steinebrunner, G., see Solca, J. 224 (1997) 253

Tran, V., see You, L. 224 (1997) 81
Trofimov, A.B. and J. Schirmer, Polarization propagator study of electronic excitation in key heterocyclic molecules. II. Furan 224 (1997) 175
Tronc, M., see Guillot, F. 224 (1997) 281

Vanderkooi, J.M., see Köhler, M. 224 (1997) 327
Von Niessen, W., see Baltzer, P. 224 (1997) 95

Wang, C.-X., see You, L. 224 (1997) 81
Wang, D.-C., see Chau, F.-T. 224 (1997) 157
Wang, L. and G.D. Billing, Molecular dynamics studies of dissociation of O_2 on Ag(111) surface 224 (1997) 65
Wannberg, B., see Baltzer, P. 224 (1997) 95
Wright, T.G., see Lee, E.P.F. 224 (1997) 191

Yang, B., see Guan, D. 224 (1997) 243
Yi, X., see Guan, D. 224 (1997) 243
You, L., Q. Liu, Y. Shi, C.-X. Wang, M. Lahaye and V. Tran, The conformational study of β-D-GlcA-(1,4)-L-Rha in solution by NMR and molecular dynamics simulations 224 (1997) 81
Yu, M., S. Kalvoda and M. Dolg, An incremental approach for correlation contributions to the structural and cohesive properties of polymers. Coupled-cluster study of *trans*-polyacetylene 224 (1997) 121

ELSEVIER

Chemical Physics 224 (1997) 341–349

Chemical Physics

Subject index to volume 224

Methods and constructs

Theoretical

Computational methods for electronic structure

Semiclassical electronic eigenvalues for charge asymmetric one-electron diatomic molecules: general method and sigma states, S.K. Knudson and I.C. Palmer 224 (1997) 1

An incremental approach for correlation contributions to the structural and cohesive properties of polymers. Coupled-cluster study of *trans*-polyacetylene, M. Yu, S. Kalvoda and M. Dolg 224 (1997) 121

Ab initio NMR chemical shieldings in the neutral and charged 7-phosphabicyclo[2.2.1]heptane, -heptene, and -heptadiene systems; the largest predicted downfield shift for a conventional organophosphorus molecule, D.B. Chesnut 224 (1997) 133

Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones, F. Pulm, J. Schramm, J. Hormes, S. Grimme and S.D. Peyerimhoff 224 (1997) 143

HeI photoelectron spectra of PH_2 and PF_2: comparison between simulation and experiment, F.-T. Chau, J.M. Dyke, E.P.F. Lee, A. Ridha and D.-C. Wang 224 (1997) 157

-CI and valence bond approach

Multireference configuration-interaction studies on the UV and photoelectron spectrum of phosgene, Cl_2CO, M.R.J. Hachey and F. Grein 224 (1997) 19

-perturbative and many body approaches

Polarization propagator study of electronic excitation in key heterocyclic molecules. II. Furan, A.B. Trofimov and J. Schirmer 224 (1997) 175

The geometric structure and stability of the $NO^+ \cdot CH_4$ cationic complex, E.P.F. Lee, P. Mack and T.G. Wright 224 (1997) 191

Single determinant calculations of excited state polarizabilities, D. Jonsson, P. Norman and H. Ågren 224 (1997) 201

-density functional theory

Immediate estimation of correlation energy for molecular systems from the partial charges on atoms in the molecule, S. Kristyán 224 (1997) 33

Semiempirical methods

Immediate estimation of correlation energy for molecular systems from the partial charges on atoms in the molecule, S. Kristyán 224 (1997) 33

Algebraic approaches
Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution, C. Muñoz-Crego and J. Santamaría 224 (1997) 215

Spin states and magnetic interactions
The manifestation of degenerate electron exchange in stimulated nuclear polarization at high magnetic fields, V.R. Gorelik, V.A. Morozov, N.N. Lukzen, E.G. Bagryanskaya and R.Z. Sagdeev 224 (1997) 229

Scattering of waves and particles
Semi-classical treatment of chemical reactions: extension to 3D wave packets, N. Marković and G.D. Billing 224 (1997) 53
A theoretical treatment for the dynamics of near-resonant charge exchange in gas–surface scattering, D. Guan, X. Yi, S. Ding, B. Yang and J.A. Olson 224 (1997) 243

Collisional and reactive molecular dynamics with non-frictional forces
A theoretical treatment for the dynamics of near-resonant charge exchange in gas–surface scattering, D. Guan, X. Yi, S. Ding, B. Yang and J.A. Olson 224 (1997) 243

Reactive molecular dynamics including dissipative processes
Molecular dynamics studies of dissociation of O_2 on Ag(111) surface, L. Wang and G.D. Billing 224 (1997) 65

Molecular dynamics of many particle systems and condensed phases
The conformational study of β-D-GlcA-(1,4)-L-Rha in solution by NMR and molecular dynamics simulations, L. You, Q. Liu, Y. Shi, C.-X. Wang, M. Lahaye and V. Tran 224 (1997) 81
Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution, C. Muñoz-Crego and J. Santamaría 224 (1997) 215
Melting curve for argon calculated from pure theory, J. Solca, A.J. Dyson, G. Steinebrunner, B. Kirchner and H. Huber 224 (1997) 253

Statistical computational methods (incl. Monte Carlo)
The application of simulated annealing to the conformational analysis of disaccharides, K.J. Naidoo and J.W. Brady 224 (1997) 263

Dynamics of structures, lattices and macromolecular conformations
The application of simulated annealing to the conformational analysis of disaccharides, K.J. Naidoo and J.W. Brady 224 (1997) 263

Fluctuations and random processes
Spectral analysis of the fluorescence quenching kinetics in micelles with probe migration, M.H. Gehlen 224 (1997) 275

Experiment

Magnetic resonances
The conformational study of β-D-GlcA-(1,4)-L-Rha in solution by NMR and molecular dynamics simulations, L. You, Q. Liu, Y. Shi, C.-X. Wang, M. Lahaye and V. Tran 224 (1997) 81

The manifestation of degenerate electron exchange in stimulated nuclear polarization at high magnetic fields, V.R. Gorelik, V.A. Morozov, N.N. Lukzen, E.G. Bagryanskaya and R.Z. Sagdeev 224 (1997) 229

-Molecular spectroscopy

Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones, F. Pulm, J. Schramm, J. Hormes, S. Grimme and S.D. Peyerimhoff 224 (1997) 143

The geometric structure and stability of the $NO^+ \cdot CH_4$ cationic complex, E.P.F. Lee, P. Mack and T.G. Wright 224 (1997) 191

X-ray absorption study of potential barrier effect in group 14 tetrachlorides ($GeCl_4$, $SnCl_4$) and group 15 trichlorides (PCl_3, $AsCl_3$), F. Guillot, C. Dézarnaud-Dandine and M. Tronc 224 (1997) 281

-visible

Single determinant calculations of excited state polarizabilities, D. Jonsson, P. Norman and H. Ågren 224 (1997) 201

Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2, J. Agreiter, M. Lorenz, A.M. Smith and V.E. Bondybey 224 (1997) 301

Photon counting and phase fluorimetry

Spectral analysis of the fluorescence quenching kinetics in micelles with probe migration, M.H. Gehlen 224 (1997) 275

Photoelectron and Auger spectroscopy

An experimental and theoretical study of the valence shell photoelectron spectrum of the benzene molecule, P. Baltzer, L. Karlsson, B. Wannberg, G. Öhrwall, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and W. von Niessen 224 (1997) 95

HeI photoelectron spectra of PH_2 and PF_2: comparison between simulation and experiment, F.-T. Chau, J.M. Dyke, E.P.F. Lee, A. Ridha and D.-C. Wang 224 (1997) 157

X-ray spectroscopy

X-ray absorption study of potential barrier effect in group 14 tetrachlorides ($GeCl_4$, $SnCl_4$) and group 15 trichlorides (PCl_3, $AsCl_3$), F. Guillot, C. Dézarnaud-Dandine and M. Tronc 224 (1997) 281

Laser induced fluorescence

Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2, J. Agreiter, M. Lorenz, A.M. Smith and V.E. Bondybey 224 (1997) 301

Effective stimulated emission and excited-state absorption cross-section spectra of poly(m-phenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) and t,t′-didecyloxy-II-distyrylbenzene, W. Holzer, A. Penzkofer, S.-H. Gong, D.D.C. Bradley, X. Long and A. Bleyer 224 (1997) 315

Nonlinear optics and spectroscopy

Effective stimulated emission and excited-state absorption cross-section spectra of poly(m-phenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) and t,t′-didecyloxy-II-distyrylbenzene, W. Holzer, A. Penzkofer, S.-H. Gong, D.D.C. Bradley, X. Long and A. Bleyer 224 (1997) 315

Influence of the pH on the pocket field of cytochrome *c* type proteins, M. Köhler, J. Friedrich, M. Laberge and J.M. Vanderkooi 224 (1997) 327

Synchrotron spectroscopies
An experimental and theoretical study of the valence shell photoelectron spectrum of the benzene molecule, P. Baltzer, L. Karlsson, B. Wannberg, G. Öhrwall, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and W. von Niessen 224 (1997) 95
X-ray absorption study of potential barrier effect in group 14 tetrachlorides ($GeCl_4$, $SnCl_4$) and group 15 trichlorides (PCl_3, $AsCl_3$), F. Guillot, C. Dézarnaud-Dandine and M. Tronc 224 (1997) 281

Atomic and molecular beam techniques
A theoretical treatment for the dynamics of near-resonant charge exchange in gas–surface scattering, D. Guan, X. Yi, S. Ding, B. Yang and J.A. Olson 224 (1997) 243

Objects

Bulk systems

Gases
Single determinant calculations of excited state polarizabilities, D. Jonsson, P. Norman and H. Ågren 224 (1997) 201

Supersonic beams
The geometric structure and stability of the $NO^+ \cdot CH_4$ cationic complex, E.P.F. Lee, P. Mack and T.G. Wright 224 (1997) 191

Liquids neat
Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution, C. Muñoz-Crego and J. Santamaría 224 (1997) 215

Liquid mixtures and solutions
The manifestation of degenerate electron exchange in stimulated nuclear polarization at high magnetic fields, V.R. Gorelik, V.A. Morozov, N.N. Lukzen, E.G. Bagryanskaya and R.Z. Sagdeev 224 (1997) 229

Crystals
Melting curve for argon calculated from pure theory, J. Solca, A.J. Dyson, G. Steinebrunner, B. Kirchner and H. Huber 224 (1997) 253

Complex fluids

-micelles
Spectral analysis of the fluorescence quenching kinetics in micelles with probe migration, M.H. Gehlen 224 (1997) 275

Polymers
An incremental approach for correlation contributions to the structural and cohesive properties of polymers. Coupled-cluster study of *trans*-polyacetylene, M. Yu, S. Kalvoda and M. Dolg 224 (1997) 121
Single determinant calculations of excited state polarizabilities, D. Jonsson, P. Norman and H. Ågren 224 (1997) 201

Surfaces
Molecular dynamics studies of dissociation of O_2 on Ag(111) surface, L. Wang and G.D. Billing 224 (1997) 65

Biological systems
The application of simulated annealing to the conformational analysis of disaccharides, K.J. Naidoo and J.W. Brady 224 (1997) 263
Influence of the pH on the pocket field of cytochrome *c* type proteins, M. Köhler, J. Friedrich, M. Laberge and J.M. Vanderkooi 224 (1997) 327

Microscopic and mesoscopic systems

Single atoms, molecules and assemblies (incl. biological)
Immediate estimation of correlation energy for molecular systems from the partial charges on atoms in the molecule, S. Kristyán 224 (1997) 33

Molecules (neutral and ionic)
Immediate estimation of correlation energy for molecular systems from the partial charges on atoms in the molecule, S. Kristyán 224 (1997) 33
The conformational study of β-D-GlcA-(1,4)-L-Rha in solution by NMR and molecular dynamics simulations, L. You, Q. Liu, Y. Shi, C.-X. Wang, M. Lahaye and V. Tran 224 (1997) 81
Ab initio NMR chemical shieldings in the neutral and charged 7-phosphabicyclo[2.2.1]heptane, -heptene, and -heptadiene systems; the largest predicted downfield shift for a conventional organophosphorus molecule, D.B. Chesnut 224 (1997) 133
HeI photoelectron spectra of PH_2 and PF_2: comparison between simulation and experiment, F.-T. Chau, J.M. Dyke, E.P.F. Lee, A. Ridha and D.-C. Wang 224 (1997) 157

-diatomic
Semiclassical electronic eigenvalues for charge asymmetric one-electron diatomic molecules: general method and sigma states, S.K. Knudson and I.C. Palmer 224 (1997) 1
Semi-classical treatment of chemical reactions: extension to 3D wave packets, N. Marković and G.D. Billing 224 (1997) 53
Molecular dynamics studies of dissociation of O_2 on Ag(111) surface, L. Wang and G.D. Billing 224 (1997) 65

-small polyatomics
Multireference configuration-interaction studies on the UV and photoelectron spectrum of phosgene, Cl_2CO, M.R.J. Hachey and F. Grein 224 (1997) 19
Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones, F. Pulm, J. Schramm, J. Hormes, S. Grimme and S.D. Peyerimhoff 224 (1997) 143

The geometric structure and stability of the $NO^+ \cdot CH_4$ cationic complex, E.P.F. Lee, P. Mack and T.G. Wright 224 (1997) 191
Single determinant calculations of excited state polarizabilities, D. Jonsson, P. Norman and H. Ågren 224 (1997) 201
X-ray absorption study of potential barrier effect in group 14 tetrachlorides ($GeCl_4$, $SnCl_4$) and group 15 trichlorides (PCl_3, $AsCl_3$), F. Guillot, C. Dézarnaud-Dandine and M. Tronc 224 (1997) 281
Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2, J. Agreiter, M. Lorenz, A.M. Smith and V.E. Bondybey 224 (1997) 301

-aromatics
An experimental and theoretical study of the valence shell photoelectron spectrum of the benzene molecule, P. Baltzer, L. Karlsson, B. Wannberg, G. Öhrwall, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and W. von Niessen 224 (1997) 95
Polarization propagator study of electronic excitation in key heterocyclic molecules. II. Furan, A.B. Trofimov and J. Schirmer 224 (1997) 175
Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution, C. Muñoz-Crego and J. Santamaría 224 (1997) 215

-polymeric and biological
An incremental approach for correlation contributions to the structural and cohesive properties of polymers. Coupled-cluster study of *trans*-polyacetylene, M. Yu, S. Kalvoda and M. Dolg 224 (1997) 121
Effective stimulated emission and excited-state absorption cross-section spectra of poly(m-phenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) and t,t′-didecyloxy-II-distyrylbenzene, W. Holzer, A. Penzkofer, S.-H. Gong, D.D.C. Bradley, X. Long and A. Bleyer 224 (1997) 315

Molecular aggregates

-dimers
Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution, C. Muñoz-Crego and J. Santamaría 224 (1997) 215

Free radicals (incl. hydronium and muonium)
The manifestation of degenerate electron exchange in stimulated nuclear polarization at high magnetic fields, V.R. Gorelik, V.A. Morozov, N.N. Lukzen, E.G. Bagryanskaya and R.Z. Sagdeev 224 (1997) 229
Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2, J. Agreiter, M. Lorenz, A.M. Smith and V.E. Bondybey 224 (1997) 301

Defects and impurities
Melting curve for argon calculated from pure theory, J. Solca, A.J. Dyson, G. Steinebrunner, B. Kirchner and H. Huber 224 (1997) 253

Proteins
Influence of the pH on the pocket field of cytochrome *c* type proteins, M. Köhler, J. Friedrich, M. Laberge and J.M. Vanderkooi 224 (1997) 327

Phenomena

Molecular structure
An incremental approach for correlation contributions to the structural and cohesive properties of polymers. Coupled-cluster study of *trans*-polyacetylene, M. Yu, S. Kalvoda and M. Dolg 224 (1997) 121
The geometric structure and stability of the $NO^+ \cdot CH_4$ cationic complex, E.P.F. Lee, P. Mack and T.G. Wright 224 (1997) 191
The application of simulated annealing to the conformational analysis of disaccharides, K.J. Naidoo and J.W. Brady 224 (1997) 263

Vibrations and rotations of molecules
Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2, J. Agreiter, M. Lorenz, A.M. Smith and V.E. Bondybey 224 (1997) 301

Surface chemical physics

-surface reactions
Molecular dynamics studies of dissociation of O_2 on Ag(111) surface, L. Wang and G.D. Billing 224 (1997) 65
A theoretical treatment for the dynamics of near-resonant charge exchange in gas–surface scattering, D. Guan, X. Yi, S. Ding, B. Yang and J.A. Olson 224 (1997) 243

Electronic structure and states
Semiclassical electronic eigenvalues for charge asymmetric one-electron diatomic molecules: general method and sigma states, S.K. Knudson and I.C. Palmer 224 (1997) 1
Multireference configuration-interaction studies on the UV and photoelectron spectrum of phosgene, Cl_2CO, M.R.J. Hachey and F. Grein 224 (1997) 19
Immediate estimation of correlation energy for molecular systems from the partial charges on atoms in the molecule, S. Kristyán 224 (1997) 33
An experimental and theoretical study of the valence shell photoelectron spectrum of the benzene molecule, P. Baltzer, L. Karlsson, B. Wannberg, G. Öhrwall, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and W. von Niessen 224 (1997) 95
Polarization propagator study of electronic excitation in key heterocyclic molecules. II. Furan, A.B. Trofimov and J. Schirmer 224 (1997) 175
X-ray absorption study of potential barrier effect in group 14 tetrachlorides ($GeCl_4$, $SnCl_4$) and group 15 trichlorides (PCl_3, $AsCl_3$), F. Guillot, C. Dézarnaud-Dandine and M. Tronc 224 (1997) 281
Effective stimulated emission and excited-state absorption cross-section spectra of poly(m-phenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) and t,t′-didecyloxy-II-distyrylbenzene, W. Holzer, A. Penzkofer, S.-H. Gong, D.D.C. Bradley, X. Long and A. Bleyer 224 (1997) 315

Critical behavior and phase transitions
Melting curve for argon calculated from pure theory, J. Solca, A.J. Dyson, G. Steinebrunner, B. Kirchner and H. Huber 224 (1997) 253

Biomolecular structure–function relationships
Influence of the pH on the pocket field of cytochrome *c* type proteins, M. Köhler, J. Friedrich, M. Laberge and J.M. Vanderkooi 224 (1997) 327

Spectral bandshapes and intensities
Theoretical and experimental investigations of the electronic circular dichroism and absorption spectra of bicyclic ketones, F. Pulm, J. Schramm, J. Hormes, S. Grimme and S.D. Peyerimhoff 224 (1997) 143

Coupling of electronic and nuclear motion
Polarization propagator study of electronic excitation in key heterocyclic molecules. II. Furan, A.B. Trofimov and J. Schirmer 224 (1997) 175

Molecular photophysical processes
An experimental and theoretical study of the valence shell photoelectron spectrum of the benzene molecule, P. Baltzer, L. Karlsson, B. Wannberg, G. Öhrwall, D.M.P. Holland, M.A. MacDonald, M.A. Hayes and W. von Niessen 224 (1997) 95
Spectral analysis of the fluorescence quenching kinetics in micelles with probe migration, M.H. Gehlen 224 (1997) 275

Photochemistry
The manifestation of degenerate electron exchange in stimulated nuclear polarization at high magnetic fields, V.R. Gorelik, V.A. Morozov, N.N. Lukzen, E.G. Bagryanskaya and R.Z. Sagdeev 224 (1997) 229

Intramolecular dynamics
Dynamical mechanism for the intermolecular relaxation of the excited NH stretching vibration of a pyrrole molecule in liquid solution, C. Muñoz-Crego and J. Santamaría 224 (1997) 215

-radiationless transitions
Neon matrix spectra and isotopically dependent fluorescence quantum yields of BO_2, J. Agreiter, M. Lorenz, A.M. Smith and V.E. Bondybey 224 (1997) 301

Luminescence spectra, yields and lifetimes
Effective stimulated emission and excited-state absorption cross-section spectra of poly(m-phenylenevinylene-co-2,5-dioctoxy-p-phenylenevinylene) and t,t′-didecyloxy-II-distyrylbenzene, W. Holzer, A. Penzkofer, S.-H. Gong, D.D.C. Bradley, X. Long and A. Bleyer 224 (1997) 315

Nonlinear responses (incl. optical)
Single determinant calculations of excited state polarizabilities, D. Jonsson, P. Norman and H. Ågren 224 (1997) 201

Reactions (incl. dissociation)

-collisional
Semi-classical treatment of chemical reactions: extension to 3D wave packets, N. Marković and G.D. Billing 224 (1997) 53

Ionization (incl. Rydberg states)
Multireference configuration-interaction studies on the UV and photoelectron spectrum of phosgene, Cl_2CO, M.R.J. Hachey and F. Grein 224 (1997) 19

Molecular motion (incl. diffusive)
Spectral analysis of the fluorescence quenching kinetics in micelles with probe migration, M.H. Gehlen 224 (1997) 275